Monte Carlo simulation of the nuclear medium: Fermi gases, nuclei and the role of Pauli potentials.

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The role of Pauli potentials in the semiclassical simulation of Fermi gases at low temperatures is investigated. An alternative Pauli potential to the usual bivariate Gaussian form by Dorso *et al*[5] is proposed. This new Pauli potential allows for a simultaneous good reproduction of not only the kinetic energy per particle but also the momentum distribution and the two-body correlation function. The reproduction of the binding energies in finite nuclei in the low and medium mass range is also analyzed. What is found is that given a reasonable short-range atractive nuclear interaction one can include correlation effects in a suitable chosen density dependent Pauli potential.

Keywords: Fermi gas, Pauli potential, many-body simulations, nuclear pasta.

1. Formalism

Nuclear many-body simulations are a useful tool to study the relevant properties of the nuclear medium in the thermodynamic conditions arising in matter in the aftermath of a Supernova event or in Neutron Stars. Examples of this are, for instance, nuclear *pastas*[1,2] at densities in the range $0.01\rho_0 \leq \rho \leq 0.5\rho_0$ ($\rho_0 = 0.148\, fm^{-3}$) and temperatures of decens of MeV or in heavy ion collisions.[3] This type of simulations based on Monte Carlo or Molecular Dynamics techniques allow for a dynamical description of the nuclear medium usually by using an effective interaction hamiltonian in a semiclassical treatment. In fermionic systems the genuine antisymmetrization of the wave function is considered trough the inclusion of a Pauli potential. Pioneering works on this line include those of Wilets*et al.*[4] In this work the hamiltonian used to study the low temperature nucleon systems consists of a kinetic energy term and a Pauli effective potential (V_{Pauli}).

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_N} + \sum_{i=1,j>i}^{A} V_{Pauli}(r_{ij}, p_{ij}) \delta_{\tau_i \tau_j} \delta_{\sigma_i \sigma_j}, \tag{1}$$

where $\delta_{\tau_i\tau_j}$ ($\delta_{\sigma_i\sigma_j}$) is the Kronecker's delta for the nucleon isospin (spin) third-component. $\mathbf{p}_i$ is the 3-momentum of i-th nucleon and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ ($p_{ij} = |\mathbf{p}_i - \mathbf{p}_j|$) the relative distance (momentum) of the i-th and j-th nucleons.

We will consider, for the sake of comparison, two ways to implement this potential.

i) A Gaussian form introduced by Dorso *et al.*,[5]

$$V_{Pauli}(r_{ij}, p_{ij}) = V_S \ \exp\left(-\frac{r_{ij}^2}{2q_0^2} - \frac{p_{ij}^2}{2p_0^2}\right), \tag{2}$$

Here p_0 and q_0 are momentum and length scales related to the excluded phase-space volume that is used to mimic fermionic correlations and V_S is the Pauli potential strength. All three parameters have been adjusted to reproduce only the kinetic energy of a low temperature Fermi gas.

ii) A new form proposed, based on spatial and momentum-dependent, two-body terms of the following form[6]

$$V_{Pauli}^{new}(r_{ij}, p_{ij}) = V_q \exp(-r_{ij}/q_0) + V_p \exp(-p_{ij}/p_0) + V_\Theta \, \Theta_\eta(q_i) \ , \tag{3}$$

where $q_i = |\mathbf{p}_i|/p_{\rm F}$, and Θ_η is a smeared Heaviside-step function, $\Theta_\eta(q) \equiv \frac{1}{1+\exp[-\eta(q^2-1)]}$ and $\Theta_\eta(q) \longrightarrow \Theta(q)$ when η is sufficiently big. The parameters of the new Pauli potential V_q, V_p, V_Θ and q_0, p_0, η will be adjusted to reproduce the kinetic energy per particle and both the momentum distribution and two-body correlation function of a low-temperature Fermi gas. The first and second terms in the potential penalize two particles with the same quantum numbers coming together either in space or momentum. This retains the essence of the fermionic wave function given by the Slater determinant. The third term forbids any particle from having a momentum significantly larger than the Fermi momentum.

In both cases the potential parameters will depend on the density of the system and this will be crucial in reproducing experimental binding energies when simulating low and medium mass nuclei as will be shown later. The values for the parameters at saturation density ρ_0 and reduced temperature $\tau = T/T_F = 0.05$ are given in Table 1.

Table 1. Pauli potential parameters.

Pauli potential	Potential strength (MeV)	q_0 (fm)	p_0 (MeV/c)
Dorso *et al*[5]	$V_S = 207$	1.644	120
This work	$V_q = 13.517$, $Vp = 1.260$, $V_\Theta = 3.560$ ($\eta = 30$)	0.66	49.03

2. Results

The simulations are performed in a NVT system with $\tau = T/T_F$, and N fermions in a cubic box of volume $V = L^3 = N/\rho$. Then, using the Metropolis algorithm the system is thermalized until the stage where configurations are sampled in order to calculate the statistical averages for the magnitudes discussed below.

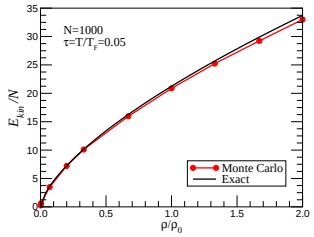

Fig. 1. Energy per particle of a Fermi gas simulated with $N = 1000$ particles at $T = 0.05T_F$ as a function of density.

In Fig. 1 the red line shows the kinetic energy per particle for a Fermi gas system with $N = 1000$ particles at $\tau = 0.05$ as a function of density calculated using the new form of the Pauli potential Eq.(3). Also plot with a black line is the exact result. We can see that there is a good reproduction of the kinetic energy.

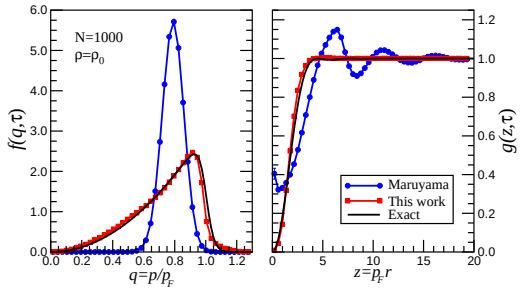

Fig. 2. Momentum distribution function and two-body correlation function of a Fermi gas. See text for details.

In Fig. 2 we can see on the left side the momentum distribution function $f(q, \tau)$ and, on the right side, the two-body correlation function $g(z, \tau)$ with $z = p_F r$. The blue curves correspond to the Dorso potential Eq.(2) and the red curves to the new Pauli potential proposed Eq.(3). Again the black line shows the exact result. We can see that a simultaneous good reproduction of both magnitudes is achieved with the alternative new potential but not with the Dorso version. Particurlarly the "Fermi hole" fails to be reproduced at small distances with the Dorso potential. This should be emphasized since these models are used in nuclear many-body simulations

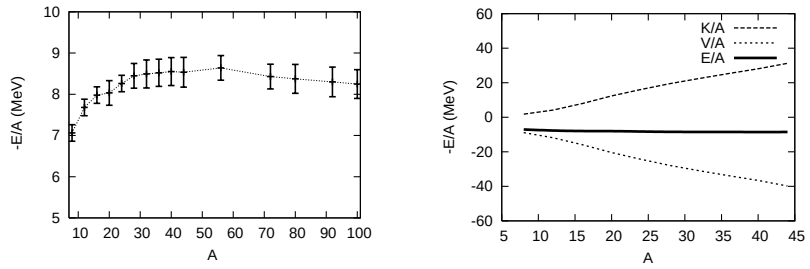

Fig. 3. Application to nuclei. (a) Binding energy. (b) Kinetic and potential contributions to the binding energy.

as in nuclear *pastas* as, for instance, in the work by Maruyama *et al.*[2] The velocity distribution,[6] not shown here, however peaks at lower values than the momentum distribution due to the fact that canonical and kinematical momentum are not the same quantities.[7] This is a genuine feature in this treatment with momentum dependent Pauli potentials in a hamiltonian formalism.

We now show finite nuclei simulation[8] results calculated with a simplified square-well nuclear potential with $V_{well} = -3$ MeV of width 2 fm and a core with $V_{core} = 10$ MeV and width 1 fm. Coulomb interaction is also included. In Fig. 3(a) binding energy per particle for a low to medium mass set of spin saturated symmetric nuclei of A nucleons. As can be seen in Fig. 3(b) kinetic(dashed line) and potential(dotted line) energy balance to obtain the total binding energy (solid line) per particle. The density dependence of the parameters of the Pauli potential is crucial to provide enough positive contribution to the linearly A-growing negative potential energy[8] and reproduce the experimental binding energy curve.

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